Nonlinear Fluid Flow/Surfactant/Interface Dynamics

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LONG-TERM GOALS

The goal of this research is the development of a theoretical quantitative understanding of the dynamics of high Reynolds number free-surface flows under large free-surface deformations in the presence of one or multiple surfactants. The long-term goal of this research is to understand the effect of the surfactants on (1) turbulence, (2) waves, (3) slick formation, and (4) mass transfer through the free surface.

OBJECTIVES

The objectives of the proposed research are several. First, we are aiming to develop an algorithm for direct numerical simulation of free-surface flows with surfactants. The scheme will be capable of simulating two-dimensional flows with high Reynolds numbers, accommodating nonlinear free-surface deformation and the presence of one or two interacting surfactants. Second, we want to use this tool to evaluate alternative approaches in modeling surfactant behavior. In particular, through comparison with experimental data, we want to investigate the extent of microscopic detail needed to be present in the surfactant model in order to enable an at least qualitative description of the dynamic surfactant behavior. We want to focus on improving the understanding of the flow/free-surface/surfactant interactions through a direct simulation of the nonlinear interactions of a surfactant-contaminated free surface with a vortex with or without the presence of waves.

APPROACH

The approach followed for the accurate and computationally efficient evaluation of the flow, free-surface deformation and surfactant concentration involves to development of a direct numerical simulation capability based on a fully spectral spatial discretization and a conformal mapping of the flow domain into a regular parallelepiped. The conformal mapping is key in order to preserve the computational efficiency of the proposed numerical technique since it allows the use of computationally efficient fast Poisson algorithms for the solution of the Poisson and Helmholtz problems generated from the time-integration of the flow and surfactant concentration evolution equations. The numerical time-integration approach can be either a mixed implicit/explicit scheme, or a fully implicit scheme. These approaches have led to very efficient numerical schemes for stationary boundary problems. The mixed integration scheme has recently been extended to three dimensions. For free-surface problems, we have developed a fully implicit scheme for simulating fully nonlinear free-surface problems. We are currently incorporating the capability to handle surfactants, which is now straightforward. In addition to this work, we have gained extensive experience in parallel computing and have the capability of performing our simulations in powerful parallel computing environments through very efficient implementations of our algorithms, which are linearly scalable

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with the number of processors. Thus, we are in a unique position to perform efficient simulations of free-surface flows with surfactants, accommodating fully nonlinear free-surface deformations, with very high accuracy.

WORK COMPLETED

During the past year, we extended significantly our algorithm for flow in channels with deformed boundaries by improving its range of applicability in three directions, retaining its almost linear scalability (the number of operations required are order $N\log_2 N$, where N is the number of unknowns):

- We successfully extended the solid boundary algorithm to incorporate a third dimension.
- We implemented two different schemes for fully implicit time integration.
- We successfully extended our two-dimensional algorithm to accommodate a free surface.

Specifically, for our three-dimensional algorithm we utilized the mixed explicit/implicit integration scheme discussed in a recent publication in the *Journal of Computational Physics* dealing with the two-dimensional case (Dimitropoulos *et al.*, 1998a), extending it through the use of a modified preconditioner used in the iterative solver. The main difficulty in the three dimensional case is the efficient implementation of the influence matrix method for satisfying the divergence-free condition. For the type of mapping used in our case (pseudoconformal mapping), the divergence now has a function (a scale factor) multiplying the third term corresponding to the spanwise direction (z), which leads to the of coupling the Fourier modes and to a non-separable equation:

$$\frac{\partial u_\xi}{\partial \xi} + M\,\frac{\partial u_\eta}{\partial \eta} + h_\xi^2\,\frac{\partial u_z}{\partial z} = 0,$$

where (ξ, η, z) are the pseudoconformal coordinates and M is the constant ratio of the scale factors along ξ and η. The scale factor along z is equal to unity. To get around this obstacle, we decided to satisfy the divergence iteratively within the preconditioner, utilizing a similar Concus and Golub type transformation as for the Navier-Stokes equations. This in principle leads to an convergent algorithm for flows which do not have dominating flow-field variations in the spanwise direction as one can see from our analysis of the basic scheme in our previous work (Dimitropoulos and Beris, 1997; Dimitropoulos *et al.*, 1998a). This algorithm is currently being validated for flows with three-dimensional flow-fields in a parallel supercomputer. Additionally, we now perform our simulations on parallel machines using MPI, where, as expected, we observe almost linear scalability of performance with the number of processors, consistent with the initial design objectives for our algorithms.

For the free-surface problem, we have observed that stability necessitates the use of fully implicit algorithms when dealing with nonlinear boundary conditions. We have implemented implicit time-integration in two different ways. First, we used second order Adams-Moulton time-integration for the nonlinear terms in the Navier-Stokes equation, which leads to nonlinear equations to be solved at each time step. We proceed to solve this system of equations by combining our algorithm with an external Newton-Raphson scheme. This is especially suited for use in problems with large contributions from the nonlinear terms. Our procedure consists of linearizing our equations and attaining the form:

$$\nabla^2(\delta\mathbf{v}) - \frac{2\,\mathrm{Re}}{\Delta t}(\delta\mathbf{v}) - 2\,\mathrm{Re}\,\nabla(\delta p) = RHS\left(t < t^{n+1}\right) + RHS\left(t^{n+1}; \mathbf{v}, p\right) + RHS\left(t^{n+1}; \delta\mathbf{v}, \delta p\right)$$

where the right-hand sides (RHS) can be thought of as a contribution belonging to the previous steps, a contribution from the current time-step which is updated at every Newton's iteration and a contribution which is updated continuously within each Newton's iteration as we solve for the corrections δq, where

q is any variable through an iterative algorithm, the preconditioned conjugate gradient algorithm described in our earlier work. This method has no problems in satisfying the divergence-free condition since each iterate is found to be divergence-free by the same influence matrix algorithm as before. The computational cost per time-step of this scheme compared to our previous algorithm for two-dimensional problems is proportional to the number of Newton-Raphson iterations used, typically around 3-5 when a decent and divergence-free initial guess is supplied.

One can also implement an implicit approach using a predictor-corrector scheme, using an Adams-Bashforth scheme for the non-linear terms in the predictor step and an Adams-Moulton scheme for the corrector step. This algorithm is only 2 times more expensive than the mixed scheme and has the advantage that the initial guess need not satisfy the continuity equation very well, allowing for more freedom. Of course, the main disadvantage compared to the full Adams-Moulton scheme using the external Newton-Raphson scheme is that it is not as stable. However, it is adequately stable for use even in free-surface problems. The concept behind the algorithm is simple. One recalculates the nonlinear terms at the current time step after the predictor step is finished and resolves with a modified right-hand side corresponding to these terms. In fact, the corrector step converges faster than the predictor step, since the iterative algorithm starts with a better initial guess. Therefore, the algorithm is actually less than a factor of 2 slower than that using a mixed time-integration scheme.

The solution of the free-surface problem was initially attempted through the use of the mixed algorithm. However, stability considerations made us abandon that scheme in favor of a predictor-corrector scheme, which can handle the problem in the least intrusive manner compared to the solid boundary code. Starting from our code for moving solid boundaries (see Dimitropoulos *et al.*, 1998a), we can implement the kinematics condition along with the orthogonality constraint in the algorithm that computes the time-derivatives of the mapping. This is achieved by solving iteratively two separable Poisson equations, using a similar method to that in Dimitropoulos *et al.* (1998a), with the following (coupled) boundary conditions:

$$\frac{\partial y}{\partial t} = \left(u_\eta - \frac{\partial x}{\partial t}\frac{\partial x}{\partial \eta} \right) \Big/ \frac{\partial y}{\partial \eta},$$

$$\frac{\partial}{\partial \eta}\left(\frac{\partial x}{\partial t}\right) = \left(-\frac{\partial}{\partial \xi}\left(\frac{\partial x}{\partial t}\right)\frac{\partial x}{\partial \eta} - \frac{\partial}{\partial \xi}\left(\frac{\partial y}{\partial t}\right)\frac{\partial y}{\partial \eta} - \frac{\partial}{\partial \eta}\left(\frac{\partial y}{\partial t}\right)\frac{\partial y}{\partial \xi} \right) \Big/ \frac{\partial x}{\partial \xi}.$$

Once the time-derivatives of the mapping are known, we can then find the actual mesh by integrating in time. To enforce orthogonality over the time-integration error, we fit the top boundary calculated through the time-integration to a Fourier series and then use this Fourier series as a functional representation in the mapping algorithm for a given surface (described in Dimitropoulos et al.*, 1998a). We then proceed to solve for the flow problem with a known mesh at the new time-step. This is made robust through a predictor-corrector scheme. Initially, we use explicit integration for the mesh. We solve for the velocities and then recalculate the time-derivatives of the mesh with this new velocity and use implicit integration for the mesh. We proceed to solve again for the velocity field. Once this first corrector step is completed, we repeat it until the values we obtain do not change. This is necessary since we have decoupled the solution of the mesh from the solution of the flow problem. This would not be possible using the fully implicit scheme with the Newton-Raphson iteration. This approach allows us to implement the full nonlinear free-surface boundary conditions without needing to change substantially the preconditioned conjugate gradient solver. The free-surface boundary conditions as expressed in the pseudoconformal coordinate system utilized in this work are:*

$$-p\,\mathrm{Re}+\frac{2M}{h_\xi^2}\left(\frac{\partial u_\eta}{\partial \eta}-\frac{\partial \ln h}{\partial \eta}u_\eta+\frac{1}{M}\frac{\partial \ln h}{\partial \xi}u_\xi\right)=\frac{2H}{Ca}\qquad \text{normal stress}$$

$$\frac{\partial u_\eta}{\partial \xi}+\frac{\partial u_\xi}{\partial \eta}-2\frac{\partial \ln h}{\partial \xi}u_\eta-2\frac{\partial \ln h}{\partial \eta}u_\xi=0\qquad \text{tangential stress,}$$

where Ca is the capillary number and H is the mean curvature of the interface. We implement these boundary conditions in the preconditioner, along with the divergence-free condition after transforming them into the following set of equations:

$$-p^i=\frac{2M}{K\,\mathrm{Re}}\left[\left(\frac{\partial u_\eta}{\partial \eta}\right)^i+\left(-\frac{\partial \ln h}{\partial \eta}u_\eta+\frac{1}{M}\frac{\partial \ln h}{\partial \xi}u_\xi-p\frac{h_\xi^2-K}{2M}\mathrm{Re}\right)^{i-1}-RBC1\right]$$

$$\left(\frac{\partial u_\xi}{\partial \eta}\right)^i=\left(-\frac{\partial u_\eta}{\partial \xi}+2\frac{\partial \ln h}{\partial \xi}u_\eta+2\frac{\partial \ln h}{\partial \eta}u_\xi\right)^{i-1}+RBC2$$

$$\left(\frac{\partial u_\eta}{\partial \eta}\right)^i=-\frac{1}{M}\left(\frac{\partial u_\xi}{\partial \xi}\right)^{i-1}+RBC3.$$

The constant K is simply the average of the square of the scale factor, RBC1, RBC2, RBC3 are the residuals of the boundary conditions calculated in the conjugate gradient level and *i* is the index of the Concus and Golub type iteration performed in the preconditioner. This scheme differs from that for the solid boundary case in that the boundary conditions change at every preconditioner iteration.

RESULTS

We present briefly a validation result for the free-surface simulation algorithm. We simulated a wave of amplitude equal to 10^{-3} in a channel 2 units deep and 1 unit wide. The Reynolds number used was 10^4 (based on half-depth and gravity), whereas the corresponding capillary number for water was 10^{-1}. The time-step was equal to 10^{-2}. This corresponds to a period of 2.55 time units. Our results agree well with the theoretical results of Levich (1960) for damping of waves with small viscosity. Figure 1 shows the time-evolution of the interface shape. Detailed results for all the work discussed in this report will be available in a series of future publications.

IMPACT/APPLICATIONS

We have extended our computationally efficient numerical scheme for solving spectrally two-dimensional, time-dependent flow problems in moderately complex geometries to accommodate implicit time-integration, a third dimension for the solid boundary case and a free-surface for the two-dimensional case. Our methods exhibit almost linear scalability and exponential convergence with mesh refinement. They use an orthogonal mapping algorithm, an efficient and robust iterative solver incorporating the influence matrix method for satisfying the incompressibility condition. In addition the algorithms are parallelizable in a straightforward fashion and exhibit linear scalability of their performance with the number of processors used. They provide unique new computational tools for the calculation of complex multidimensional and time-dependent flows, such as free-surface flows with surfactants, turbulent flow over irregular (albeit smooth) boundaries, blood flow in arteries and polymer resin flow in model porous media, which is of importance to composite manufacturing. We are currently extending the free-surface code for simulation of free-surface flows with surfactants, where we solve the fully coupled nonlinear problem of fluid flow and mass transport of the surfactant.

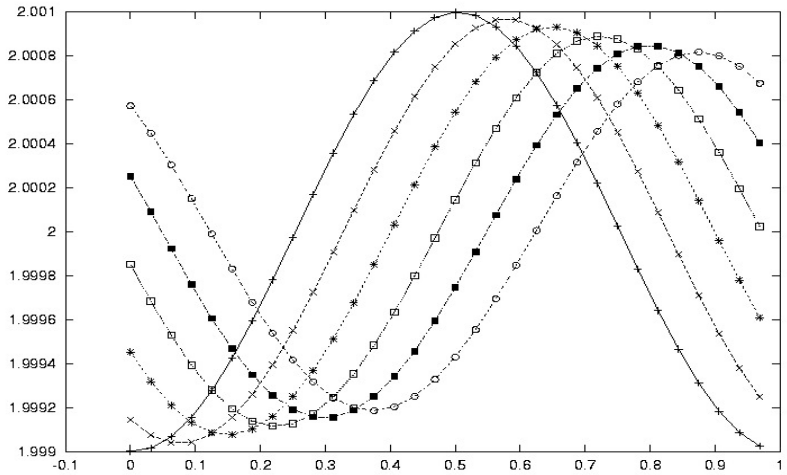

Figure 1: Evolution in time of the interface shape of a small-amplitude, large-wavelength water wave.

TRANSITIONS

The main development of this work is a quite general in applicability algorithm, which extends the use of full spectral methods to flows within moderately complex geometries. The tools developed in this work i.e. the pseudoconformal mapping and the efficient spectral preconditioner are also applicable to other computational fluid mechanics and transport phenomena problems. All of these are expected to find significant use within the computational fluid dynamics community, since their possible applications span a quite wide area.

RELATED PROJECTS

The core of the spectral numerical method, after suitable modification, has been successfully used in direct numerical simulations (DNS) of multidimensional and time-dependent viscoelastic flows in a joint University of Delaware - NRL effort for the investigation of polymer-induced turbulent drag reduction. We have gained significant experience in parallel computing from this project, since we have performed extensive simulations on the CRAY T3D, T3E systems at the Pittsburgh Supercomputing Center (PSC) and the CRAY-Origin2000 at National Center for Supercomputing Applications (NCSA). This work has led to a publication discussing our first calculations in *Physics of Fluids* (Sureshkumar et al., 1997) and another in the *Journal of Non-Newtonian Fluid Mechanics* (Dimitropoulos *et al.*, 1998b), where the effect of rheology in polymer-induced drag reduction is examined. The transfer of the codes developed in the current project from the single-processor to multiple-processor environments has been greatly facilitated from the above-mentioned experience.

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